

Supporting Information:

Energy landscape and phase competition of CsV₃Sb₅, CsV₆Sb₆ and TbMn₆Sn₆-type Kagome materials

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Guanghui Cai and Yutao Jiang contributed equally to this work.

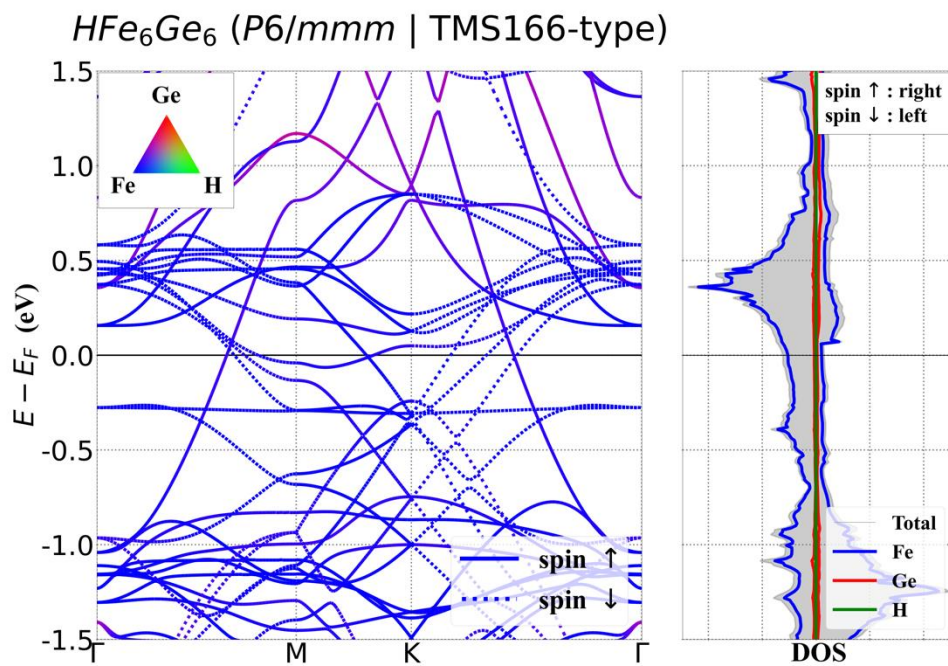
Table.S1: List of 89 compounds with high thermal stability ($E_{\text{hull}} < 20\text{meV/atom}$). The first column represents the chemical formula, the second column represents the structure type, the third column represents the id of the compound in atomly.net, the fourth column represents the E_{hull} (meV/atom) of the compound.

Chemical Formula	Structure type	Atomly ID	E_{hull}(meV/atom)
HMn ₆ Ge ₆	TMS166	1000301627	14.97
HFe ₆ Sn ₆	TMS166	1000301639	11.18
HFe ₆ Ge ₆	TMS166	1000301638	0.00
HCo ₆ Sn ₆	TMS166	1000301650	7.65
HCo ₆ Ge ₆	TMS166	1000301649	0.00
HNi ₆ Sn ₆	TMS166	1000301661	0.68
HRh ₆ Pb ₆	TMS166	1000301728	17.64
HRh ₆ Sn ₆	TMS166	1000301727	3.35
LiTi ₆ Bi ₆	TMS166	1000301823	4.84
LiTi ₆ Pb ₆	TMS166	1000301827	17.44
LiTi ₆ Sb ₆	TMS166	1000301822	17.49
LiV ₆ Sn ₆	TMS166	1000301837	10.59

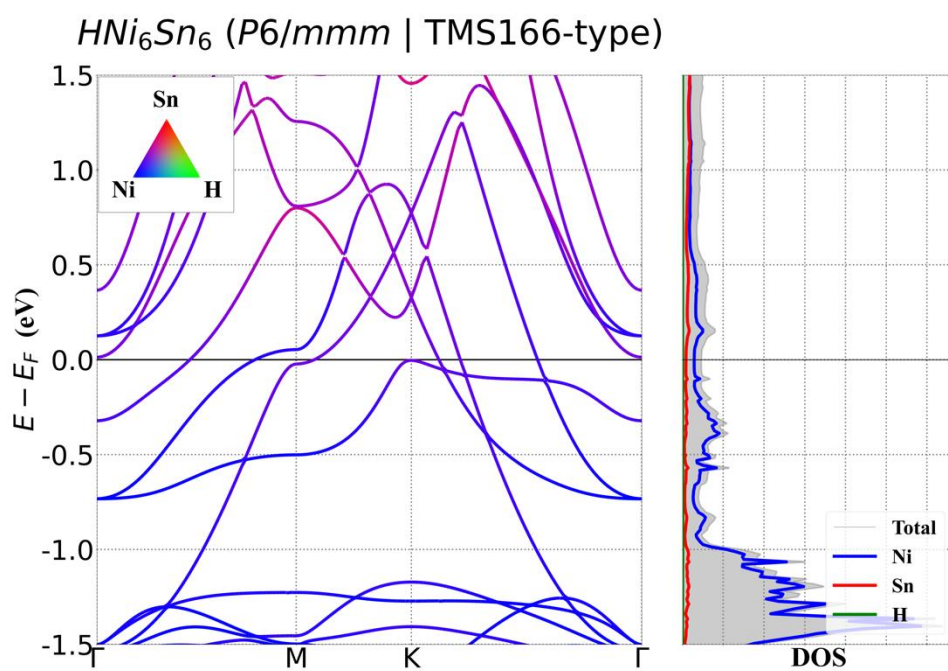
LiMn ₆ Sn ₆	TMS166	1000301858	18.35
LiMn ₆ Ge ₆	TMS166	3001812095	0.00
LiFe ₆ Ge ₆	TMS166	3001812096	0.00
LiCo ₆ Ge ₆	TMS166	0000060277	0.00
LiNi ₆ Sn ₆	TMS166	1000301888	12.78
LiNi ₆ Ge ₆	TMS166	0000043146	0.00
LiNi ₆ Si ₆	TMS166	0000102969	2.72
LiTc ₆ Ge ₆	TMS166	1000301931	16.04
NaTi ₃ Bi ₅	CVS135	1000299281	0.00
NaTi ₆ Bi ₆	TMS166	1000302050	6.42
NaV ₃ Sb ₅	CVS135	1000299291	2.02
NaMn ₃ Sb ₅	CVS135	1000299313	6.69
NaMn ₆ Ge ₆	TMS166	1000302085	13.22
NaFe ₆ Ge ₆	TMS166	1000302096	6.55
NaCo ₆ Ge ₆	TMS166	3001812089	6.78
NaRh ₆ Pb ₆	TMS166	1000302186	4.79
NaRh ₆ Sn ₆	TMS166	1000302185	0.00
NaPd ₆ Pb ₆	TMS166	1000302197	0.00
NaPd ₆ Sn ₆	TMS166	1000302196	13.39
KTi ₃ Bi ₅	CVS135	1000299512	0.00
KTi ₆ Bi ₆	CVS166	1000300902	3.79
KV ₃ Sb ₅	CVS135	1000299522	0.00
KV ₆ Sb ₆	CVS166	1000300934	13.37
KMn ₃ Sb ₅	CVS135	1000299544	0.00
KFe ₆ Sb ₆	CVS166	1000301033	8.40
KFe ₃ Sn ₅	CVS135	1000299559	18.79
KNb ₃ Bi ₅	CVS135	1000299600	0.00
KNb ₆ Bi ₆	CVS166	1000300946	9.55
KTc ₆ Sb ₆	CVS166	1000301011	9.57
KHf ₃ Bi ₅	CVS135	1000299666	2.99
RbTi ₃ Bi ₅	CVS135	1000299743	0.00
RbTi ₆ Bi ₆	CVS166	1000301133	4.08
RbTi ₃ Te ₅	CVS135	1000299750	5.13
RbTi ₃ Sb ₅	CVS135	1000299742	11.25
RbV ₃ Sb ₅	CVS135	1000299753	0.00
RbV ₆ Sb ₆	CVS166	1000301165	11.97
RbCr ₆ As ₆	CVS166	1000301197	12.13
RbMn ₃ Sb ₅	CVS135	1000299775	0.00
RbFe ₆ Sb ₆	CVS166	1000301264	0.00
RbNi ₃ Bi ₅	CVS135	1000299809	14.15
RbNb ₃ Bi ₅	CVS135	1000299831	0.00
RbNb ₆ Bi ₆	CVS166	1000301177	9.82
RbTc ₆ Sb ₆	CVS166	1000301242	0.00

RbRh ₃ Pb ₅	CVS135	1000299879	9.43
RbPd ₆ Bi ₆	CVS166	1000301342	14.65
RbHf ₃ Bi ₅	CVS135	1000299897	0.00
RbTa ₃ Sb ₅	CVS135	1000299907	18.77
CsTi ₃ Bi ₅	CVS135	1000299974	0.00
CsTi ₆ Bi ₆	CVS166	1000301364	4.48
CsTi ₃ Te ₅	CVS135	1000299981	0.00
CsTi ₃ Sb ₅	CVS135	1000299973	0.00
CsV ₃ Bi ₅	CVS135	1000299985	13.88
CsV ₃ Sb ₅	CVS135	1000299984	0.00
CsV ₆ Sb ₆	CVS166	1000301396	11.96
CsCr ₆ As ₆	CVS166	1000301428	8.77
CsMn ₃ Sb ₅	CVS135	1000300006	0.00
CsMn ₆ As ₆	CVS166	1000301461	14.91
CsMn ₃ Ge ₅	CVS135	1000300009	11.28
CsFe ₆ Sb ₆	CVS166	1000301495	0.00
CsFe ₃ Sn ₅	CVS135	1000300021	0.00
CsFe ₆ As ₆	CVS166	1000301494	16.74
CsFe ₃ Ge ₅	CVS135	1000300020	0.20
CsNi ₃ Sn ₅	CVS135	1000300043	18.00
CsZr ₃ Bi ₅	CVS135	1000300051	12.41
CsZr ₃ Te ₅	CVS135	1000300058	0.00
CsNb ₃ Bi ₅	CVS135	1000300062	0.00
CsNb ₆ Bi ₆	CVS166	1000301408	8.58
CsTc ₆ Sb ₆	CVS166	1000301473	0.00
CsTc ₆ Ge ₆	CVS166	1000301468	0.00
CsRh ₃ Pb ₅	CVS135	1000300110	0.00
CsRh ₆ Pb ₆	CVS166	1000301536	16.19
CsPd ₆ Bi ₆	CVS166	1000301573	9.65
CsPd ₃ Pb ₅	CVS135	1000300121	0.00
CsPd ₆ Pb ₆	CVS166	1000301569	1.00
CsHf ₃ Bi ₅	CVS135	1000299897	0.00
CsHf ₃ Te ₅	CVS135	1000300135	0.00
CsTa ₃ Sb ₅	CVS135	1000300138	2.27

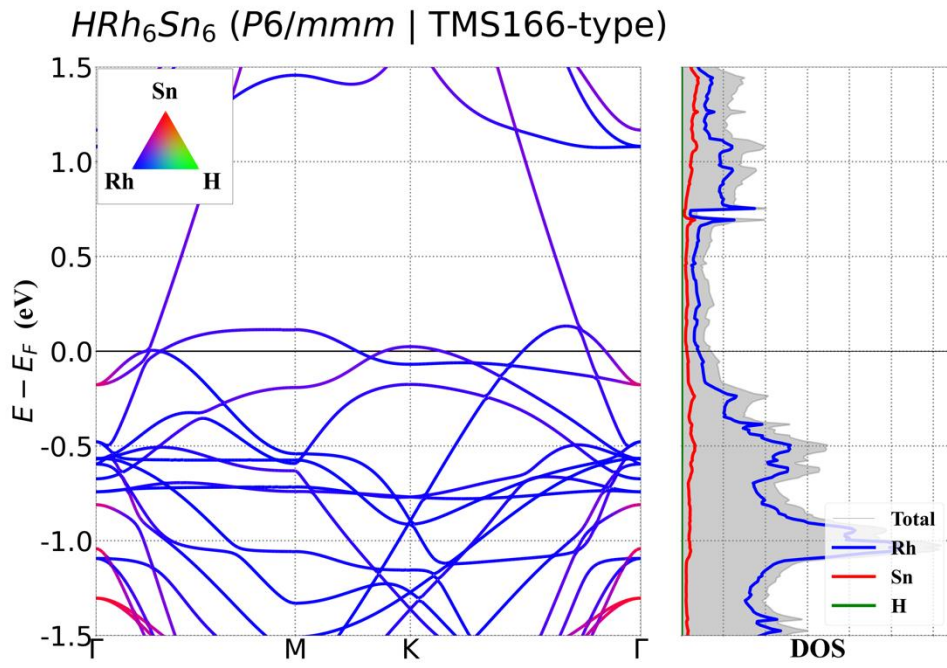
Fig.S1: The rest of band structure of TMS166 compounds with E_{hull} less than 5meV/atom.



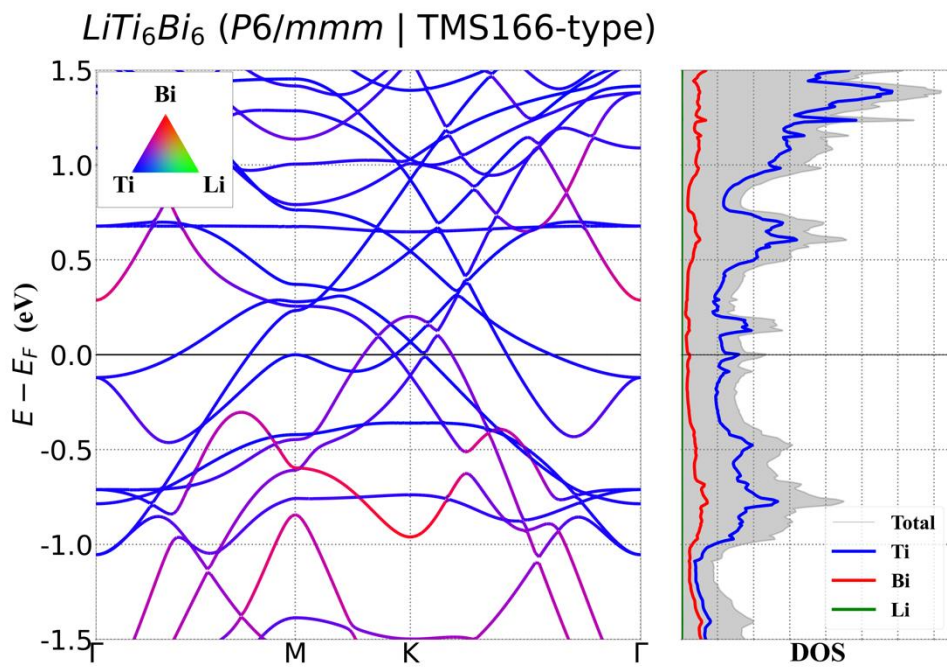
(a) HFe_6Ge_6 , Atomly ID: 1000301638



(b) HNi_6Sn_6 , Atomly ID: 1000301661

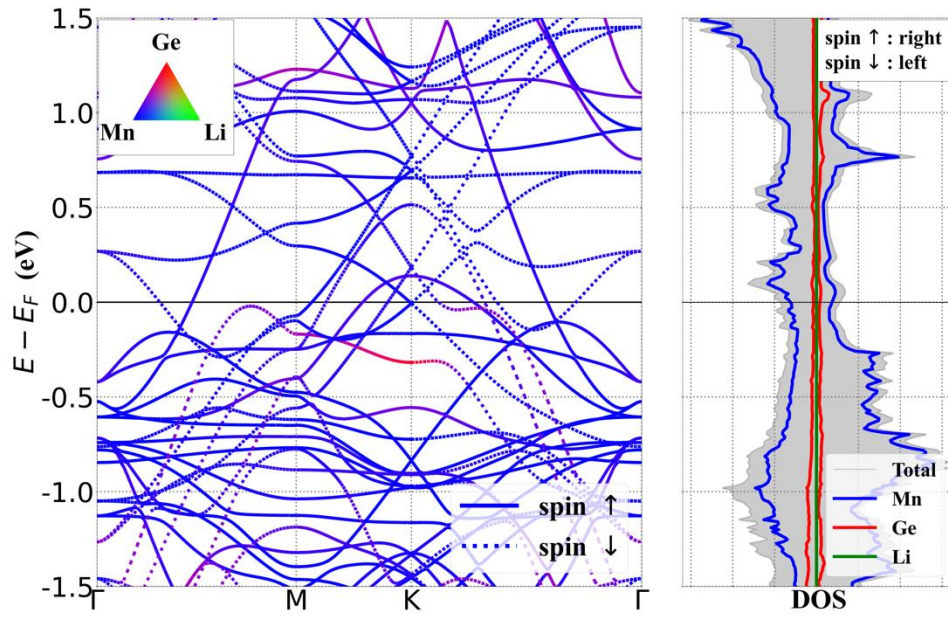


(c) HRh_6Sn_6 , Atomly ID: 1000301727



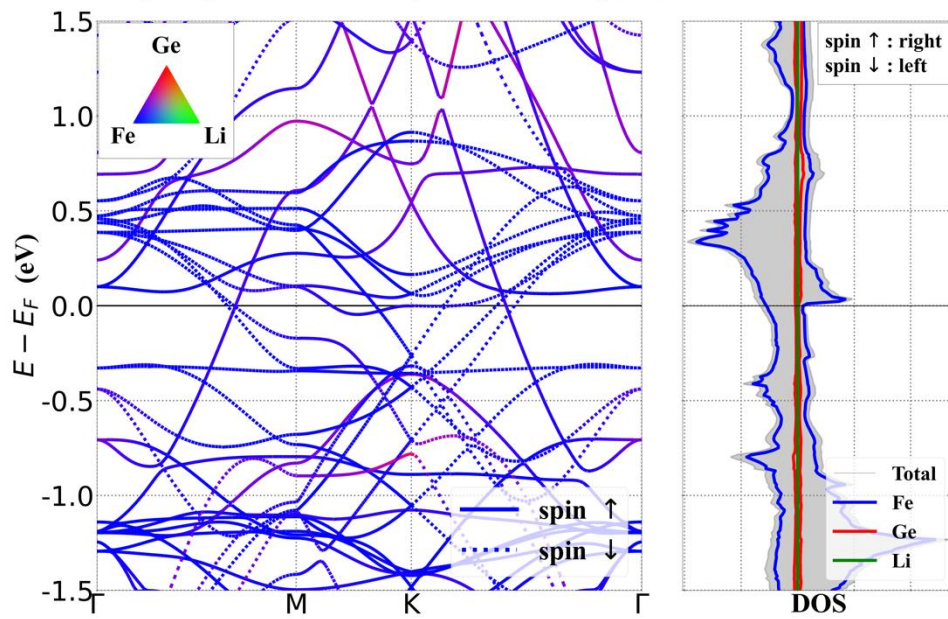
(d) LiTi_6Bi_6 , Atomly ID: 1000301823

LiMn₆Ge₆ (P6/mmm | TMS166-type)



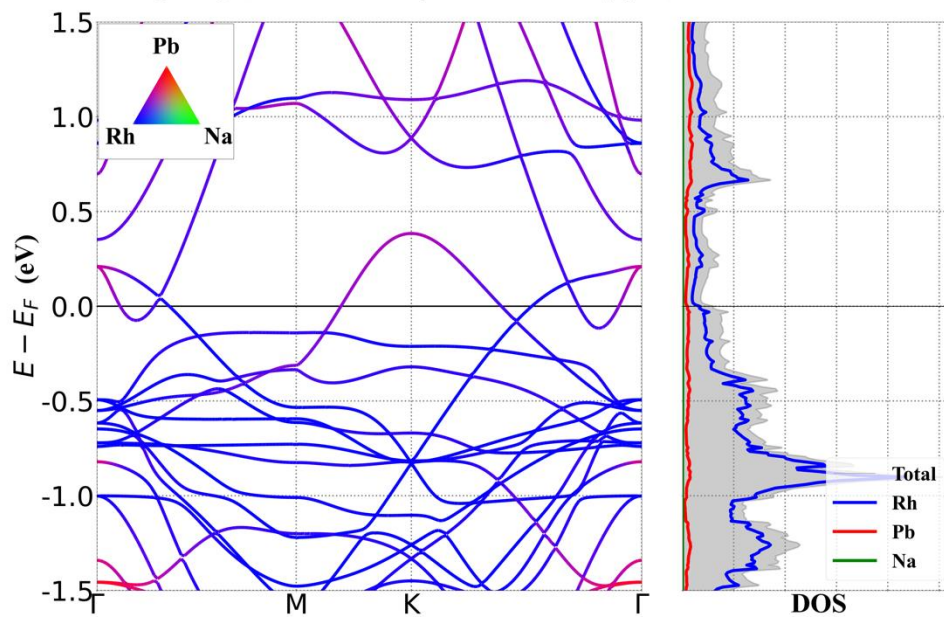
(e) *LiMn₆Ge₆*, Atomly ID: 3001812095

LiFe₆Ge₆ (P6/mmm | TMS166-type)



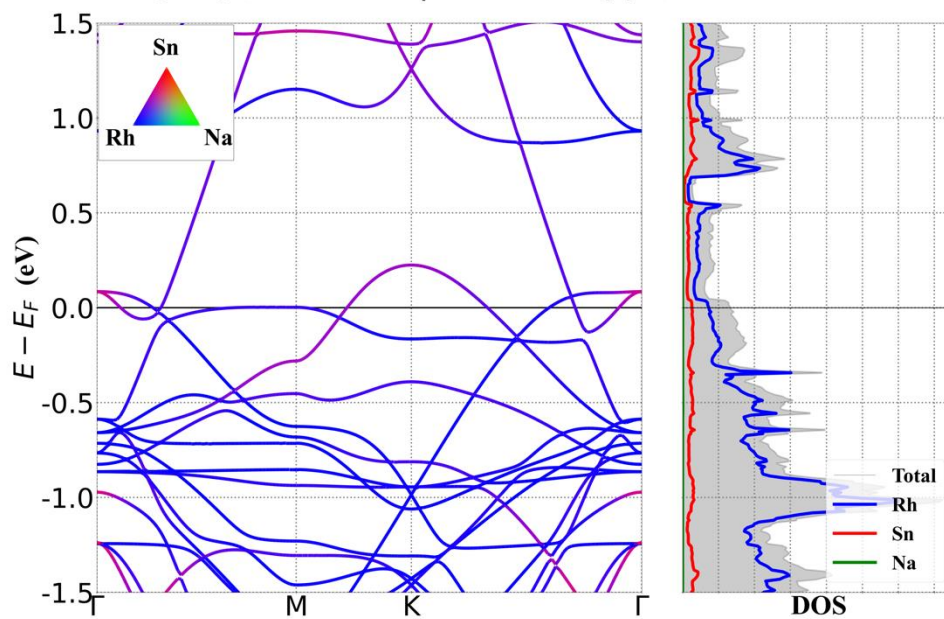
(f) *LiFe₆Ge₆*, Atomly ID: 3001812096

NaRh_6Pb_6 ($P6/mmm$ | TMS166-type)

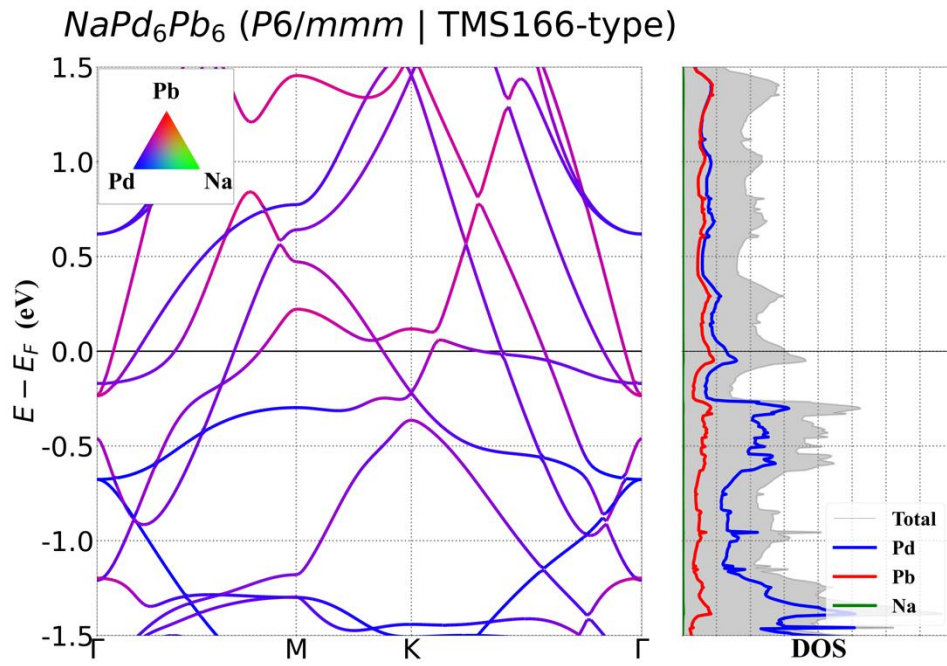


(g) NaRh_6Pb_6 , Atomly ID: 1000302186

NaRh_6Sn_6 ($P6/mmm$ | TMS166-type)

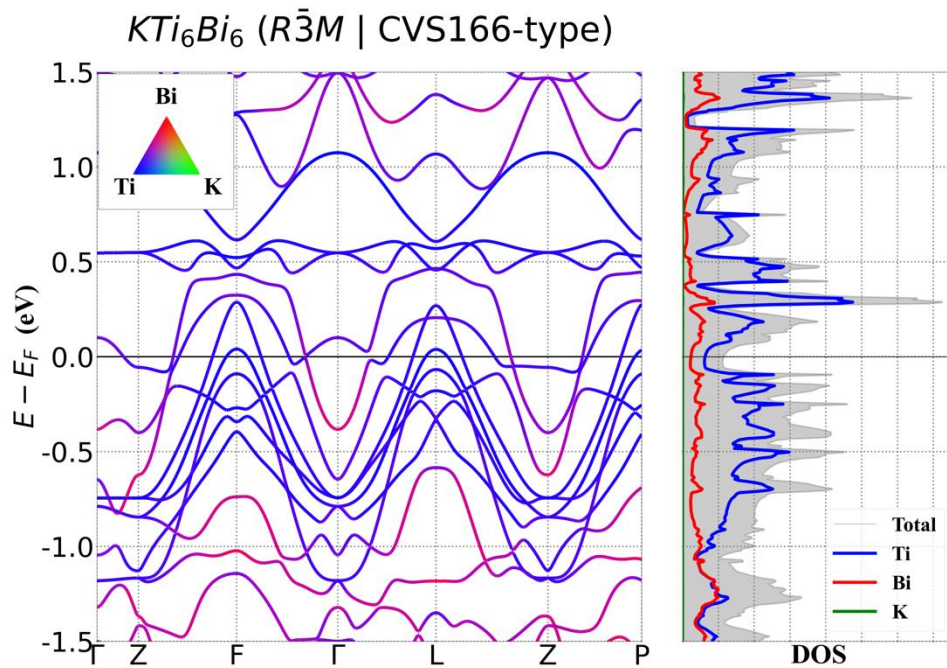


(h) NaRh_6Sn_6 , Atomly ID: 1000302185

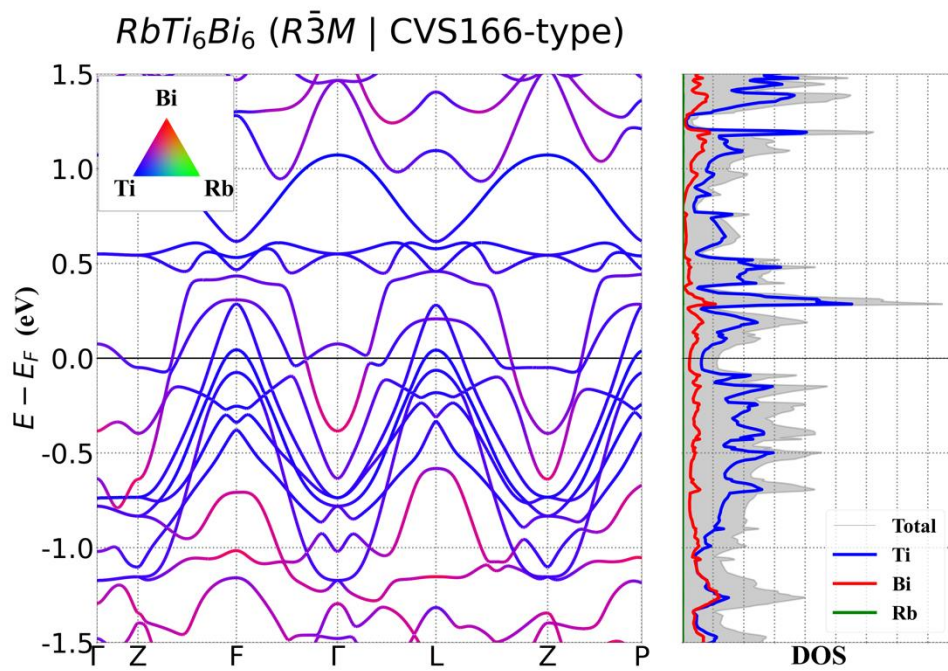


(i) NaPd₆Pb₆, Atomly ID: 1000302197

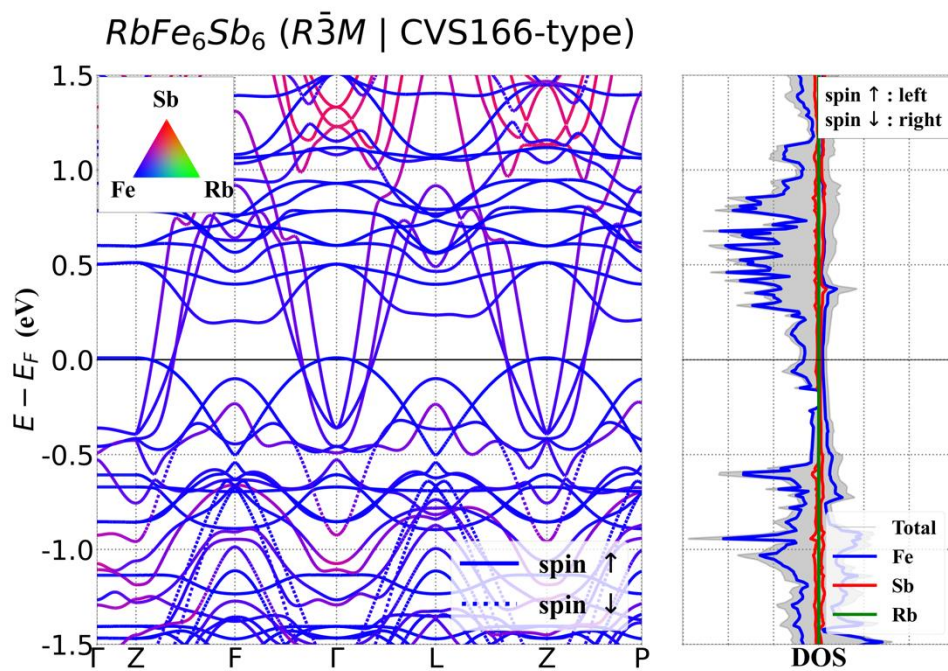
Fig.S2: The rest of band structure of CVS166 compounds with E_{hull} less than 5meV/atom.



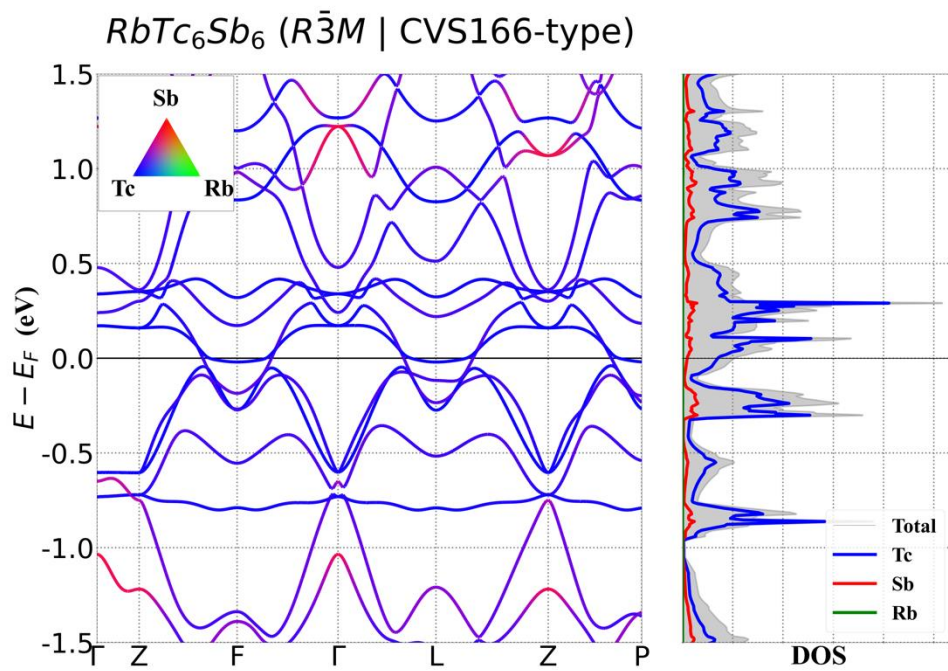
(a) KTi₆Bi₆, Atomly ID: 1000300902



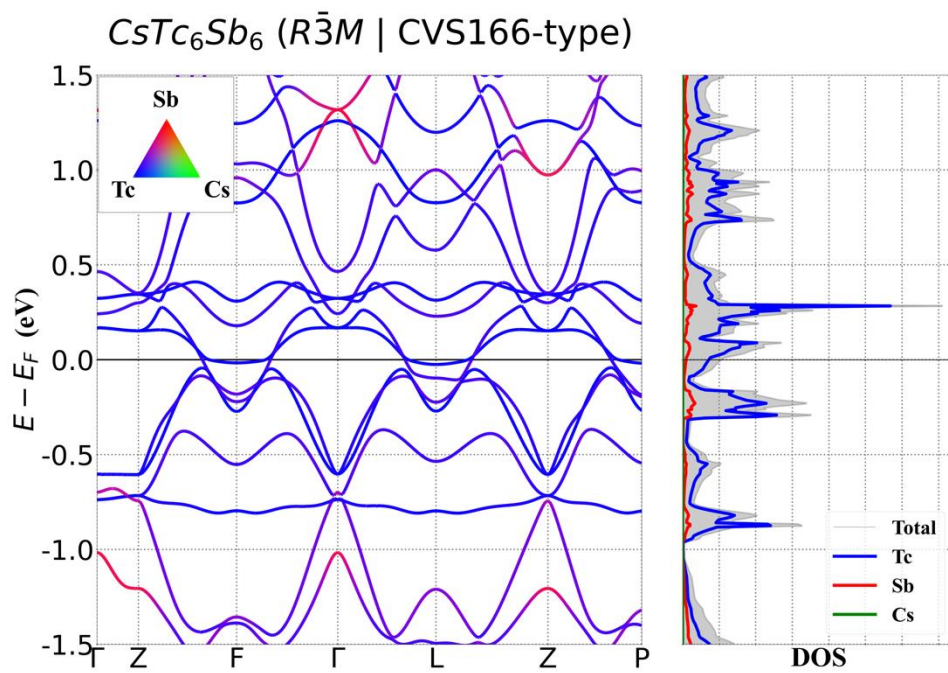
(b) $RbTi_6Bi_6$, Atomly ID: 1000301133



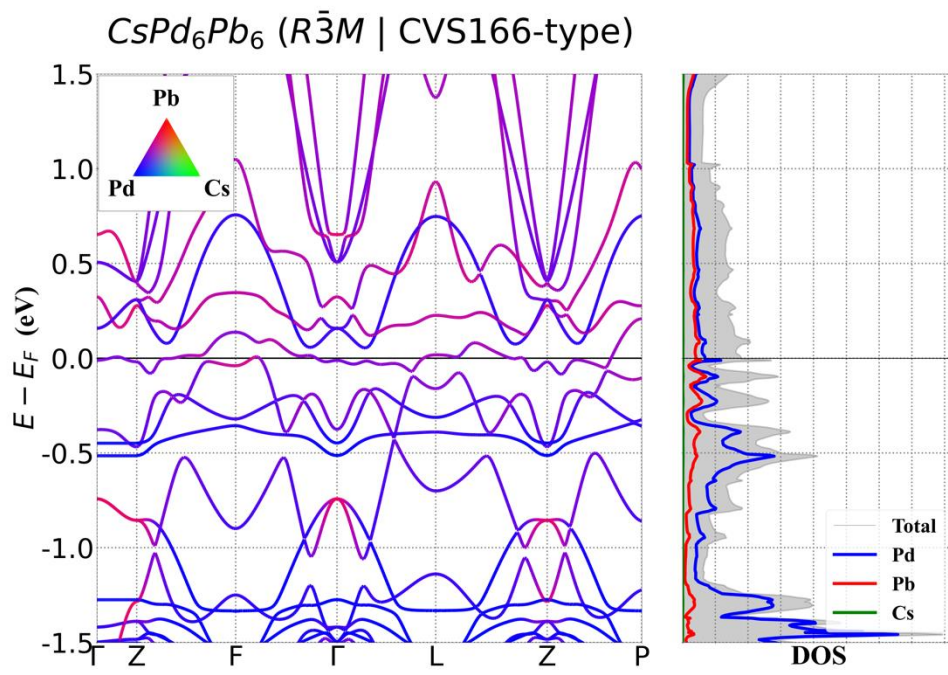
(c) $RbFe_6Sb_6$, Atomly ID: 1000301264



(d) $RbTc_6Sb_6$, Atomly ID: 1000301242



(e) $CsTc_6Sb_6$, Atomly ID: 1000301473



(f) $CsPd_6Sb_6$, Atomly ID: 1000301569